Property Prediction for Emulsion based Chemical Product Design

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Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

Property Prediction for Emulsion based Chemical Product Design

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1. INTRODUCTION

- Chemical industry is shifting from commodities towards higher value added products
- Higher value products gain their value from a molecular or micro-structure
- Product design aims to find a product exhibiting a set of desirable or specified behaviour
- Experimental data are often scarce

→Chemical product design is getting more and more important
→Modeling of emulsions becomes relevant
→Large availability of properties is required
→Predictive property models are needed

2. PURE COMPONENT PROPERTIES

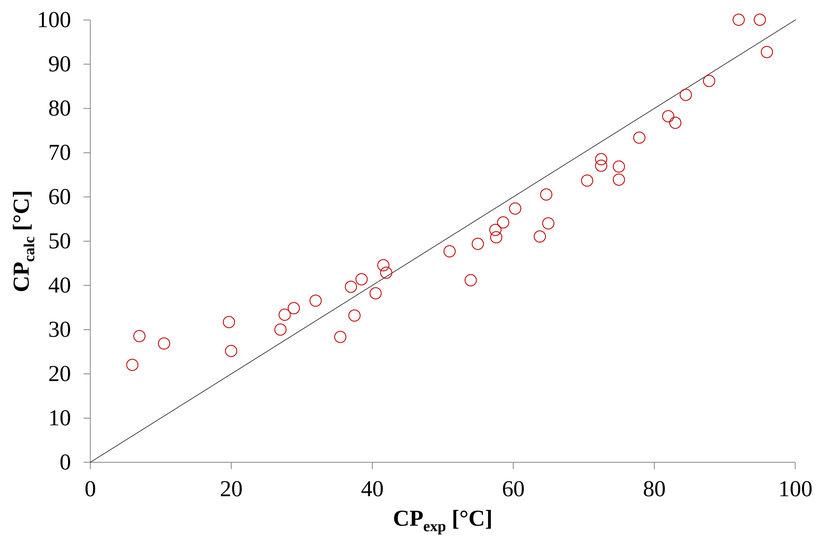
- For all components
  - Predictive models for the main properties required by a methodology for product design (viscosity, density, surface tension, solubility parameters, *etc.*) have been already developed
- **For surfactants only**
  - **Predictive models for the perculiar properties of surfactants (critical micelle concentration, cloud point, hydrophilic-lipophilic balance or equivalent, Krafft temperature, *etc.*) are missing**

3. CLOUD POINT – Original M&G GC+ method

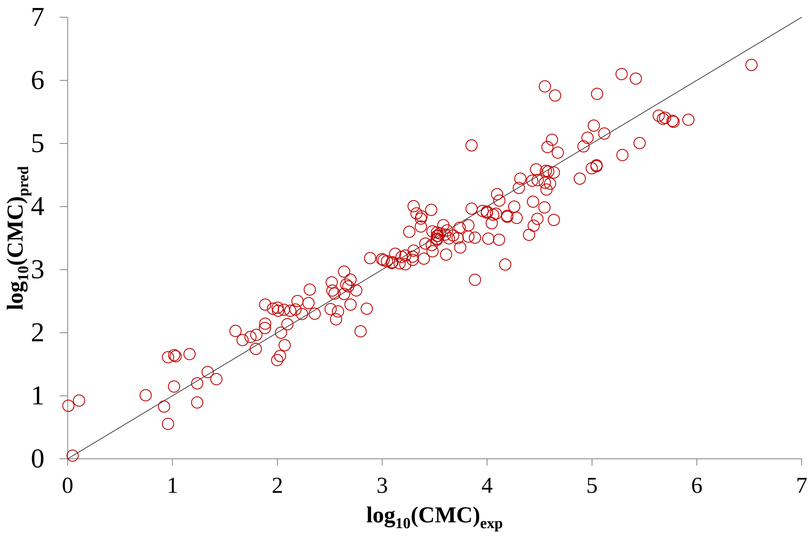
- Original M&G GC+ method

$$f(X) = \sum_i N_i C_i + w \sum_j M_j D_j + z \sum_k O_k E_k$$

- 39 experimental values
  Non-ionic surfactants, 1% w/w
- 1st order group defintion:
  4 groups
- 2nd order group defintion:
  1 group
- 3rd order group definition:
  0 groups
- R^2 = 0,85

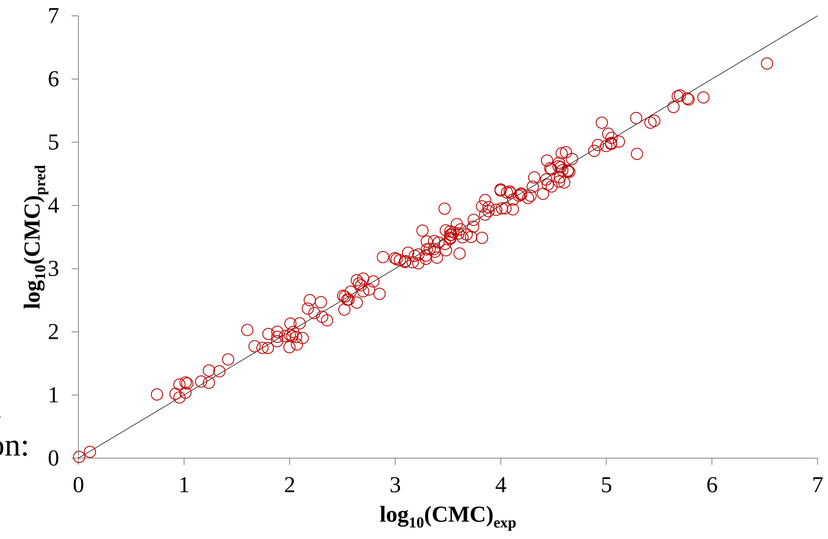


4. CRITICAL MICELLE CONCENTRATION – Extended M&G GC+ method



- Original M&G GC+ method
- 158 experimental values
  Non-ionic surfactants, 25°C
- 1st order group definition:
  34 groups
- 2nd order group definition:
  13 groups
- 3rd order group defintion:
  0 groups
- R^2 = 0,91

- Extended M&G GC+ method
- New 3rd order group definition:
  28 groups
- R^2 = 0,99

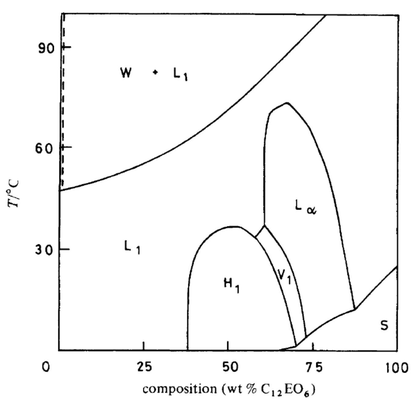


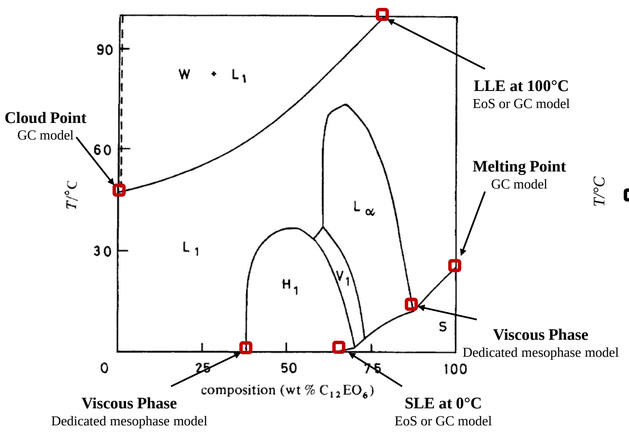
5. MIXTURE PROPERTIES

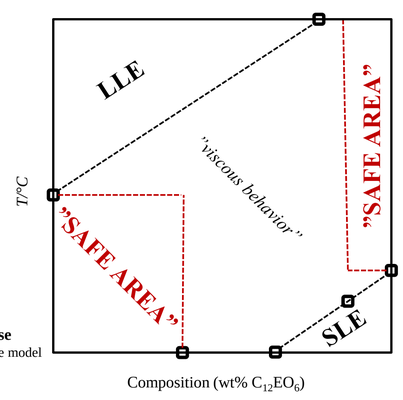
- Predictive models for mixture properties (viscosity, density, surface tension, solubility parameters, *etc.*) when considering separately the continuous and the dispersed phases have already been developed
- Predictive models for mixture properties when considering the two phases together have already been partly developed (density, cost, safety and toxicity parameters, Hansen and Hildebrand solubility parameters, evaporation time)
- **Predictive models for mixture properties when considering the two phases together are misssing (i.e. emulsion structure, viscosity, interfacial tension)**

6. WATER-SURFACTANT PHASE BEHAVIOR

- The phase diagram between water and C12EO6 is considered
- Key-points of the diagram have been identified and defined
- By measuring or predicting a few key-points, it is possible to identify ”safe areas”







7. CONCLUSIONS

- M&G GC+ methods are suitable to predict peculiar properties of non-ionic surfactants
- The addition of new dedicated third order groups can give considerable improvements
- A new third order group derfinition will be determined analyzing all the surfactant properties simultaneously
- Water-surfactant phase behavior has been reduced of complexity, by defining two safe areas, identified by 6 data-points

- New surfactant properties need to be considered, inculding ionic surfactants
- Dedicated models for interfacial tension and viscosity need to be developed
- Stability and production will be considered

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